

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 SEP 09 CA/CAPLUS records now contain indexing from 1907 to the present  
NEWS 4 Jul 15 Data from 1960-1976 added to RDISCLOSURE  
NEWS 5 Jul 21 Identification of STN records implemented  
NEWS 6 Jul 21 Polymer class term count added to REGISTRY  
NEWS 7 Jul 22 INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available  
NEWS 8 AUG 05 New pricing for EUROPATFULL and PCTFULL effective August 1, 2003  
NEWS 9 AUG 13 Field Availability (/FA) field enhanced in BEILSTEIN  
NEWS 10 AUG 15 PATDPAFULL: one FREE connect hour, per account, in September 2003  
NEWS 11 AUG 15 PCTGEN: one FREE connect hour, per account, in September 2003  
NEWS 12 AUG 15 RDISCLOSURE: one FREE connect hour, per account, in September 2003  
NEWS 13 AUG 15 TEMA: one FREE connect hour, per account, in September 2003  
NEWS 14 AUG 18 Data available for download as a PDF in RDISCLOSURE  
NEWS 15 AUG 18 Simultaneous left and right truncation added to PASCAL  
NEWS 16 AUG 18 FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation  
NEWS 17 AUG 18 Simultaneous left and right truncation added to ANABSTR  
NEWS 18 SEP 22 DIPPR file reloaded  
NEWS 19 SEP 25 INPADOC: Legal Status data to be reloaded  
NEWS 20 SEP 29 DISSABS now available on STN  
  
NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 06:47:41 ON 01 OCT 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 06:47:47 ON 01 OCT 2003

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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2  
DICTIONARY FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STNote 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

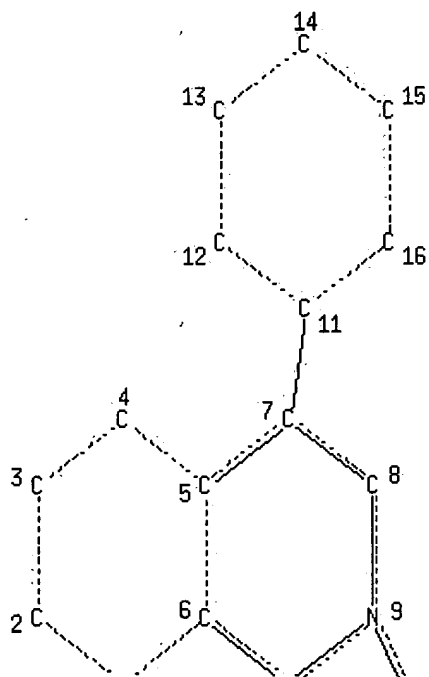
=>

L1 STRUCTURE UPLOADED

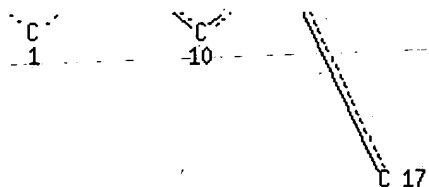
=> d 11

L1 HAS NO ANSWERS

L1 STR



Page 1-A



Page 2-A

NODE ATTRIBUTES:

NSPEC IS R AT 1  
 NSPEC IS R AT 2  
 NSPEC IS R AT 3  
 NSPEC IS R AT 4  
 NSPEC IS R AT 5  
 NSPEC IS R AT 6  
 NSPEC IS R AT 7  
 NSPEC IS R AT 8  
 NSPEC IS R AT 9  
 NSPEC IS R AT 10  
 NSPEC IS R AT 11  
 NSPEC IS R AT 12  
 NSPEC IS R AT 13  
 NSPEC IS R AT 14  
 NSPEC IS R AT 15  
 NSPEC IS R AT 16  
 NSPEC IS C AT 17  
 DEFAULT MLEVEL IS ATOM  
 MLEVEL IS CLASS AT 17  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 11  
 NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 06:49:43 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 2851 TO ITERATE

35.1% PROCESSED 1000 ITERATIONS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

42 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 53818 TO 60222  
 PROJECTED ANSWERS: 1738 TO 3050

L2 42 SEA SSS SAM L1

=>

L3 STRUCTURE UPLOADED

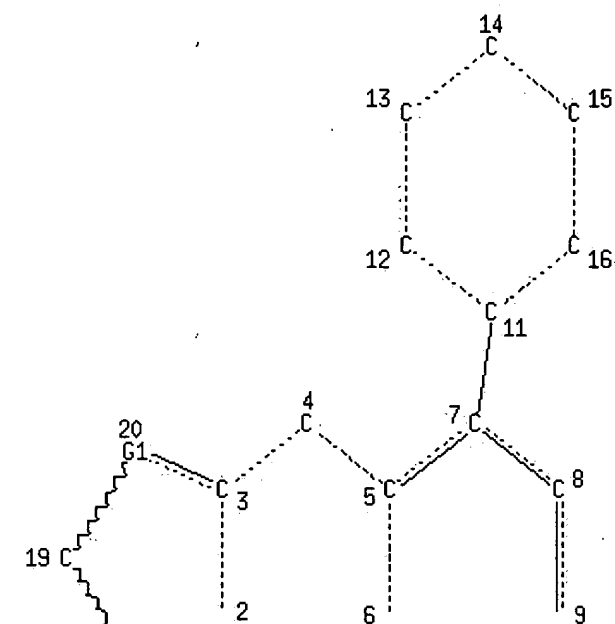
=> d 13

L3 HAS NO ANSWERS

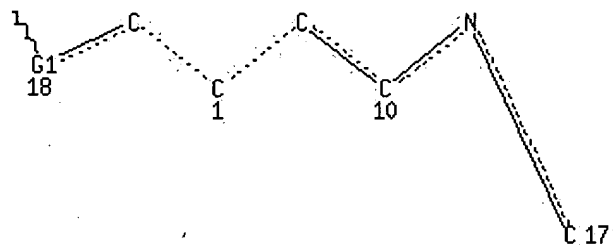
L3 STR

0 21 S 22 N 23

Page 1-A



Page 1-B



Page 2-B

VAR G1=21/22/23

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS R	AT	14
NSPEC	IS R	AT	15
NSPEC	IS R	AT	16
NSPEC	IS C	AT	17
NSPEC	IS R	AT	18
NSPEC	IS R	AT	19
NSPEC	IS R	AT	20

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 17

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 11

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

=> s 13

SAMPLE SEARCH INITIATED 06:51:40 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 660 TO ITERATE

100.0% PROCESSED 660 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 11659 TO 14741  
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=> s 13 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 06:51:44 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 13126 TO ITERATE

100.0% PROCESSED 13126 ITERATIONS 5 ANSWERS  
SEARCH TIME: 00.00.01

L5 5 SEA SSS FUL L3

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	150.55	150.76

FILE 'HCAPLUS' ENTERED AT 06:51:49 ON 01 OCT 2003  
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FILE COVERS 1907 - 1 Oct 2003 VOL 139 ISS 14  
FILE LAST UPDATED: 30 Sep 2003 (20030930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15

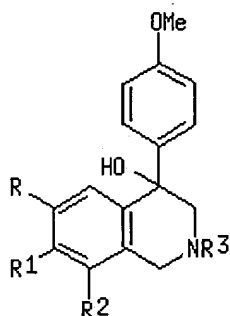
L6 5 L5

=> d 16, ibib abs fhitr, 1-5

L6 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
-----------	-------------------

ACCESSION NUMBER: 1996:613920 HCAPLUS  
 DOCUMENT NUMBER: 125:275613  
 TITLE: A convenient synthesis of 1,2,3,4-tetrahydro-4-arylisoquinolin-4-ol derivatives  
 AUTHOR(S): Coskun, Necdet; Sumengen, Dogan  
 CORPORATE SOURCE: Department Chemistry, Uludag University, Bursa, 16059, Turk.  
 SOURCE: Chimica Acta Turcica (1996), 24(2), 151-154  
 CODEN: CATUA9; ISSN: 0379-5896  
 PUBLISHER: Istanbul Universitesi, Muhendislik Fakultesi  
 Dekanligi, Kimya Muhendisligi Bolumu  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB N-Benzylaminoacetophenones were obtained by reductive amination of arom. aldehydes with amines in the presence of KBH<sub>4</sub> and alkylation with  $\alpha$ -haloacetophenones using K<sub>2</sub>CO<sub>3</sub> as a base. The title compds. I [R = R<sub>1</sub> = OMe, R<sub>2</sub> = H, R<sub>3</sub> = Me, CH<sub>2</sub>Ph; RR<sub>1</sub> = OCH<sub>2</sub>O, R<sub>2</sub> = H, R<sub>3</sub> = Me; R = H, R<sub>1</sub> = R<sub>2</sub> = OMe, R<sub>3</sub> = Me] were obtained by cyclizing the benzylaminoacetophenones with 95% H<sub>2</sub>SO<sub>4</sub> in methylene chloride.

IT 182575-15-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of arylisoquinolinols)

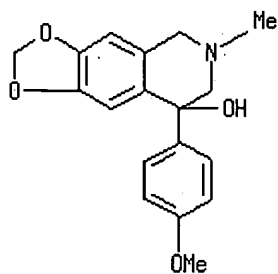
RN 182575-15-1 HCAPLUS

CN 1,3-Dioxolo[4,5-g]isoquinolin-8-ol, 5,6,7,8-tetrahydro-8-(4-methoxyphenyl)-6-methyl-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 182575-14-0

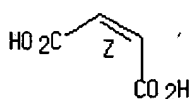
CMF C18 H19 N O4



CM 2

CRN 110-16-7  
CMF C4 H4 O4

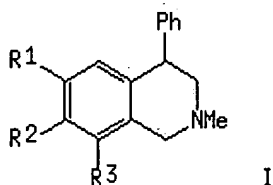
Double bond geometry as shown.



L6 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER:	1990:497422 HCAPLUS
DOCUMENT NUMBER:	113:97422
TITLE:	A new synthesis of 1,2,3,4-tetrahydro-2-methyl-4-phenylisoquinolines
AUTHOR(S):	Venkov, A.; Vodenicharov, D.
CORPORATE SOURCE:	Dep. Chem., Univ. Plovdiv, Plovdiv, 4000, Bulg.
SOURCE:	Synthesis (1990), (3), 253-5
	CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 113:97422
GI	



AB 1,2,3,4-Tetrahydro-2-methyl-4-phenylisoquinolines I (R1 = R2 = OMe, R3 = H; R1 = OH, R2 = OMe, R3 = H; R1 = H, R2 = R3 = OMe; R1 = R3 = H, R2 = OMe; R1 = OMe, R2 = R3 = H; R1 = R2 = H, R3 = H, NH2; R1R2 = OCH2O, R3 = H) are obtained from arom. aldehydes R1R2R3C6H2CHO, MeNH2, and  $\alpha$ -haloacetophenones in the presence of NaBH4 followed by cyclization with H2SO4 and Zn in MeOH.

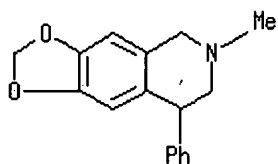
IT 128942-67-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 128942-67-6 HCAPLUS

CN 1,3-Dioxolo[4,5-g]isoquinoline, 5,6,7,8-tetrahydro-6-methyl-8-phenyl-

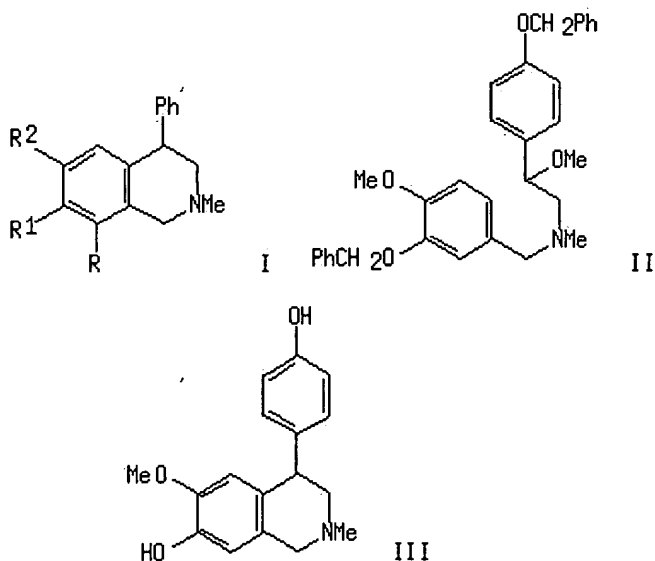
(9CI) (CA INDEX NAME)



L6 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1986:406658 HCAPLUS  
 DOCUMENT NUMBER: 105:6658  
 TITLE: Studies on tetrahydroisoquinolines. XXV. A synthesis of 4-aryl-1,2,3,4-tetrahydroisoquinolines; total synthesis of (±)-cherylline  
 AUTHOR(S): Hara, Hiroshi; Shirai, Ryuichi; Hoshino, Osamu; Umezawa, Bunsuke  
 CORPORATE SOURCE: Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan  
 SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(8), 3107-12  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 105:6658  
 GI



AB Four 4-phenyl-1,2,3,4-tetrahydroisoquinolines I (R = H, R1 = HO, R2 = MeO; R = H, R1 = MeO, R2 = HO; R = H, R1R2 = OCH2O; R = HO, R1 = MeO, R2 = H) were prep'd. from two simple synthons, styrene oxide and the corresponding benzylamines, via the β-hydroxyphenethylamines in high yield. On the other hand, β-methoxyphenethyl methanesulfonate, obtained from 4-benzyloxystyrene oxide, was coupled with a benzylamine to give the N-benzyl-β-methoxyphenethylamine II. A facile total synthesis of (±)-cherylline (III) was accomplished by acid treatment of II.



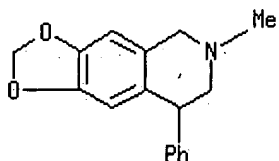
4'-O-Methylcherylline was also synthesized through the same pathway.

IT **128942-67-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN **128942-67-6** HCAPLUS

CN **1,3-Dioxolo[4,5-g]isoquinoline, 5,6,7,8-tetrahydro-6-methyl-8-phenyl-**  
(9CI) (CA INDEX NAME)



L6 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1984:85962 HCAPLUS

DOCUMENT NUMBER: 100:85962

TITLE: A facile synthesis of 4-aryl-1,2,3,4-tetrahydroisoquinolines: a total synthesis of (+)-cherylline

AUTHOR(S): Hara, Hiroshi; Shirai, Ryuichi; Hoshino, Osamu; Umezawa, Bunsuke

CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Tokyo, Tokyo, 162, Japan

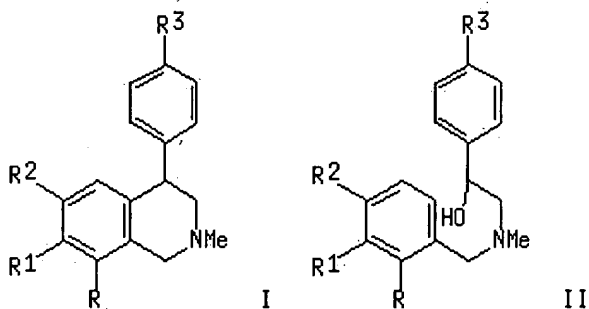
SOURCE: Heterocycles (1983), 20(10), 1945-50

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



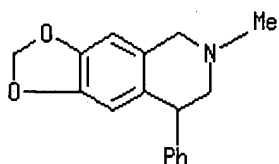
AB Cherylline (I, R = H, R1 = R3 = HO, R2 = MeO) and the related isoquinolines I [R, R1, R2, R3 = H, HO, MeO, H; HO, MeO, H, H; H, MeO, HO, H; H, HO, MeO, MeO; H, OCH2O (R2R3), H] were prepd. by cyclization of (benzylamino)phenylethanols II by treatment with acid. II were prepd. by reaction of benzylamines and styrene oxides.

IT **128942-71-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN **128942-71-2** HCAPLUS

CN **1,3-Dioxolo[4,5-g]isoquinoline, 5,6,7,8-tetrahydro-6-methyl-8-phenyl-, hydrochloride** (9CI) (CA INDEX NAME)

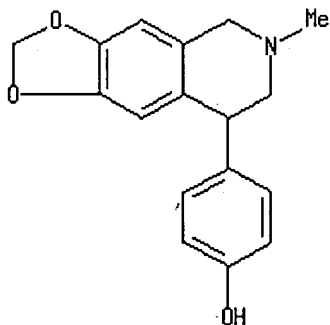


# HCl

L6 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1975:410538 HCAPLUS  
 DOCUMENT NUMBER: 83:10538  
 TITLE: Syntheses of heterocyclic compounds. DXCI. Total synthesis of (+)-cherylline and corgoine through quinonoid intermediates  
 AUTHOR(S): Kametani, Tetsuji; Takahashi, Keiichi; Chu Van Loc  
 CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, Japan  
 SOURCE: Tetrahedron (1975), 31(3), 235-8  
 CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB 3,4-(PhCH<sub>2</sub>O)(MeO)C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>NHMe at 100° for 3.5 hr with 4-PhCH<sub>2</sub>OC<sub>6</sub>H<sub>4</sub>CH(OMe)CH<sub>2</sub>Br gave 3,4-(PhCH<sub>2</sub>O)(MeO)C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>NMeCH<sub>2</sub>CH(OMe)C<sub>6</sub>H<sub>4</sub>OCH<sub>2</sub>Ph-4 which on cyclization followed by debenzoylation gave (±)-cherylline (I). Cherylline analogs II and III were prepd. similarly. Heating p-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>OH with the isoquinoline IV in a current of N gave 44% corgoine (V).  
 IT **55708-71-9P**  
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)  
 RN **55708-71-9** HCAPLUS  
 CN Phenol, 4-(5,6,7,8-tetrahydro-6-methyl-1,3-dioxolo[4,5-g]isoquinolin-8-yl)-(9CI). (CA INDEX NAME)



=&gt;

L7 STRUCTURE UPLOADED

=&gt; file reg'

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

ENTRY

29.44

TOTAL

SESSION

180.20

-3.26

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DICTIONARY FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

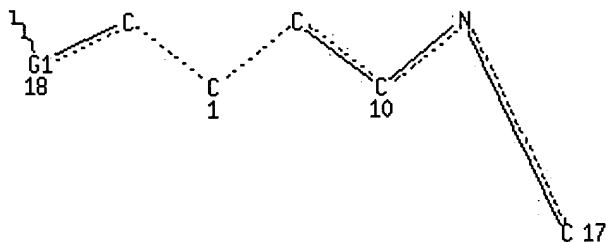
L8            STRUCTURE    UPLOADED

L8 HAS NO ANSWERS

0 04 C 00 N 03 C 04

—





Page 2-B

VAR G1=21/22/23/24

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS R	AT	14
NSPEC	IS R	AT	15
NSPEC	IS R	AT	16
NSPEC	IS C	AT	17
NSPEC	IS R	AT	18
NSPEC	IS R	AT	19
NSPEC	IS R	AT	20

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 17

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 11

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

=> s 18

SAMPLE SEARCH INITIATED 06:53:34 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 354 TO ITERATE

100.0% PROCESSED 354 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 5952 TO 8208

PROJECTED ANSWERS: 3 TO 163

L9

3 SEA SSS SAM L8

=> s 18 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 06:53:39 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 7315 TO ITERATE

100.0% PROCESSED 7315 ITERATIONS 31 ANSWERS  
 SEARCH TIME: 00.00.01

L10 31 SEA SSS FUL L8

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	148.15	328.35
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.26

FILE 'HCAPLUS' ENTERED AT 06:53:43 ON 01 OCT 2003  
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FILE COVERS 1907 - 1 Oct 2003 VOL 139 ISS 14  
 FILE LAST UPDATED: 30 Sep 2003 (20030930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 110

L11 6 L10

=> d his

(FILE 'HOME' ENTERED AT 06:47:41 ON 01 OCT 2003)

FILE 'REGISTRY' ENTERED AT 06:47:47 ON 01 OCT 2003

L1 STRUCTURE UPLOADED  
 L2 42 S L1  
 L3 STRUCTURE UPLOADED  
 L4 0 S L3  
 L5 5 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 06:51:49 ON 01 OCT 2003

L6 5 S L5  
 L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 06:53:19 ON 01 OCT 2003

L8 STRUCTURE UPLOADED

L9 3 S L8  
L10 31 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 06:53:43 ON 01 OCT 2003

L11 6 S L10

=> s l11 not l6

L12 1 L11 NOT L6

=> d l12, ibib abs fhitr, 1

1 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE  
The answer numbers requested are not in the answer set.  
ENTER ANSWER NUMBER OR RANGE (1):0  
NUMBERS IN RANGE MUST BE GREATER THAN ZERO.  
An answer number must be a positive number.  
ENTER ANSWER NUMBER OR RANGE (1):end

=> d l12, ibib abs fhitr, 1

L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 2002:51467 HCAPLUS

DOCUMENT NUMBER: 136:118393

TITLE: Preparation and use of furan-fused-4-phenyl  
substituted tetrahydroisoquinolines for treatment of  
attention deficit hyperactivity disorder (ADHD)

INVENTOR(S): Beck, James P.; Pechulis, Anthony D.; Harms, Arthur E.

PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

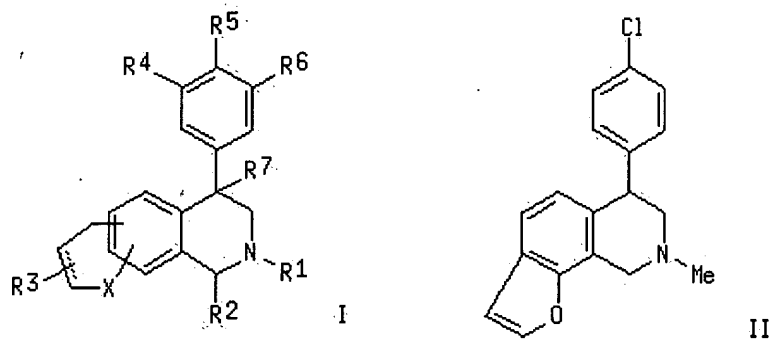
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004455	A2	20020117	WO 2001-US21818	20010711
WO 2002004455	A3	20020620		
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 2002091134	A1	20020711	US 2001-902845	20010711
EP 1299393	A2	20030409	EP 2001-952616	20010711
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2001012350	A	20030624	BR 2001-12350	20010711
PRIORITY APPLN. INFO.:			US 2000-217412P	P 20000711
			WO 2001-US21818	W 20010711

OTHER SOURCE(S): MARPAT 136:118393

GI



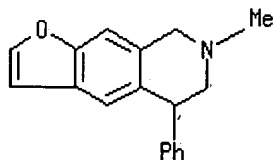
AB Title compds. I [R1 = alk(en/yn)yl, cycloalkyl, 5-cycloalkylalkyl and benzyl, each of which is optionally substituted with 1 to 3 substituents; R2 = H, alk(en/yn)yl, cycloalkyl, cycloalkylalkyl and haloalkyl; R3 = H, halo, alkyl, haloalkyl and cycloalkyl, wherein alkyl, haloalkyl and cycloalkyl are optionally substituted with 1 to 3 substituents selected from alkoxy and amino; R4-6 = H, halo, alkoxy, NO<sub>2</sub>, amino, amido, ureido, S(O)<sub>n</sub>, CN, acyl, carboxy, carboxamide, alk(en/yn)yl, cycloalkyl and cycloalkylalkyl; alternatively R5-6 = O-alkyl-O; R7 = H, halo and alkoxy; X = O, NH (and substituted derivs.) and S; n = 0 - 2] with some provisos, were prepd. E.g., 7-formylbenzofuran was converted to the corresponding methylamino-Me deriv. (MeOH, MeNH<sub>2</sub>, NaBH<sub>4</sub>), alkylated with p-chlorophenacyl bromide (CH<sub>2</sub>Cl<sub>2</sub>, Et<sub>3</sub>N) and reduced to the amino alc. (CH<sub>2</sub>Cl<sub>2</sub>, NaBH<sub>4</sub>, 5 h, 0° → room temp.). This intermediate was treated dropwise with MeOH (CH<sub>2</sub>Cl<sub>2</sub>, 0°C → reflux, overnight) to give II as a yellow oil (18% overall yield). Over 150 synthetic examples were provided. Compds. I are selective neurotransmitter receptor binding ligands (no data). I are useful in the treatment of attention-deficit hyperactivity disorder.

IT **389845-75-4P**

RL: BYP (Byproduct); PREP (Preparation)  
(byproduct; prepn. and use of furan-fused-4-Ph substituted tetrahydroisoquinolines for treatment of attention deficit hyperactivity disorder (ADHD))

RN **389845-75-4** HCAPLUS

CN Furo[3,2-g]isoquinoline, 5,6,7,8-tetrahydro-7-methyl-5-phenyl- (9CI) (CA INDEX NAME)

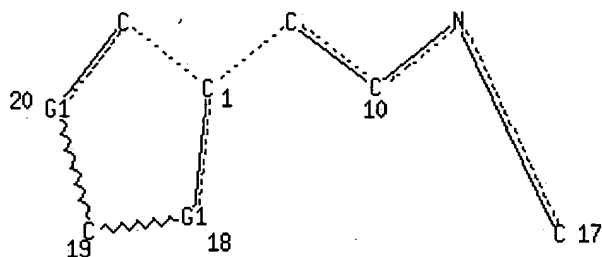


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	ENTRY	SESSION
FULL ESTIMATED COST	9.05	337.40
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.65	-3.91







Page. 2-B

VAR G1=21/22/23/24

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MLEVEL IS CLASS AT 17 21 22 23 24

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 11

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

=> s 113

SAMPLE SEARCH INITIATED 06:56:43 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 263 TO ITERATE

100.0% PROCESSED 263 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED-ITERATIONS:- 4287 TO 6233

PROJECTED ANSWERS: 8 TO 329

L14

8 SEA SSS SAM L13

=> s 113 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

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 FULL SCREEN SEARCH COMPLETED - 5253 TO ITERATE

100.0% PROCESSED 5253 ITERATIONS  
 SEARCH TIME: 00.00.01

137 ANSWERS

L15 ,137 SEA SSS FUL L13

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

148.95

486.35

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-3.91

FILE 'HCAPLUS' ENTERED AT 06:56:51 ON 01 OCT 2003  
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FILE COVERS 1907 - 1 Oct 2003 VOL 139 ISS 14  
 FILE LAST UPDATED: 30 Sep 2003 (20030930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l15

L16 2 L15

=> d l16, ibib abs fhitr, 1-2

L16 ANSWER '1 OF 2 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2002:51467 HCAPLUS

DOCUMENT NUMBER: 136:118393

TITLE: Preparation and use of furan-fused-4-phenyl substituted tetrahydroisoquinolines for treatment of attention deficit hyperactivity disorder--(ADHD)--

INVENTOR(S): Beck, James P.; Pechulis, Anthony D.; Harms, Arthur E.

PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

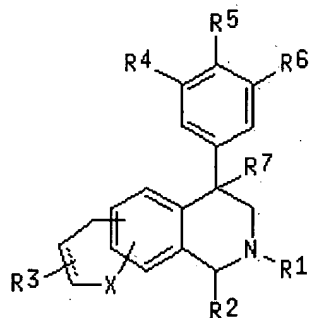
DOCUMENT TYPE: Patent

LANGUAGE: English

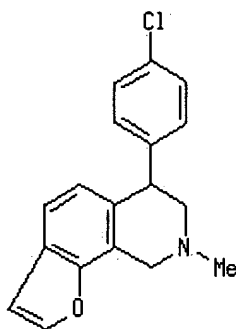
FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2002004455	A3	20020620		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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OTHER SOURCE(S): MARPAT 136:118393				
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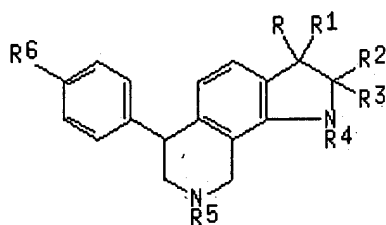
I



II

AB Title compds. I [R1 = alk(en/yn)yl, cycloalkyl, 5-cycloalkylalkyl and benzyl, each of which is optionally substituted with 1 to 3 substituents; R2 = H, alk(en/yn)yl, cycloalkyl, cycloalkylalkyl and haloalkyl; R3 = H, halo, alkyl, haloalkyl and cycloalkyl, wherein alkyl, haloalkyl and cycloalkyl are optionally substituted with 1 to 3 substituents selected from alkoxy and amino; R4-6 = H, halo, alkoxy, NO<sub>2</sub>, amino, amido, ureido, S(O)<sub>n</sub>, CN, acyl, carboxy, carboxamide, alk(en/yn)yl, cycloalkyl and cycloalkylalkyl; alternatively R5-6 = O-alkyl-O; R7 = H, halo and alkoxy; X = O, NH (and substituted derivs.) and S; n = 0 - 2] with some provisos, were prepd. E.g., 7-formylbenzofuran was converted to the corresponding methylamino-Me deriv. (MeOH, MeNH<sub>2</sub>, NaBH<sub>4</sub>), alkylated with p-chlorophenacyl bromide (CH<sub>2</sub>Cl<sub>2</sub>, Et<sub>3</sub>N) and reduced to the amino alc. (CH<sub>2</sub>Cl<sub>2</sub>, NaBH<sub>4</sub>, 5 h, 0° → room temp.). This intermediate was treated dropwise with MeOH (CH<sub>2</sub>Cl<sub>2</sub>, 0°C → reflux, overnight) to give II as a yellow oil (18% overall yield). Over 150 synthetic examples were provided. Compds. I are selective neurotransmitter receptor binding ligands (no data). I are useful in the treatment of attention-deficit hyperactivity disorder.

IT 389844-44-4P



AB The title compds. (I; R = H, alkyl aminoalkyl, heterocyclalkyl; RR1 = O, OCH2CH2O, SCH2CH2S; RR3 = atoms required to complete a 6-membered N-contg. ring; R1R2 = H, bond; R2R3 = O; R2R4 = bond; R4 = H, alkyl, iminomethyl, heterocyclalkyl; R5 = H, alkyl; R6 = halo) were prepd. Thus, 2-H2NC6H4CH2NMeCH2CHPhOH was condensed with Cl3CCH(OH)2 and HONH2.HCl to give 91% 2-HON:CHCONHC6H4CH2NMeCH2CHPhOH. This was cyclized by stirring at 35° in concd. H2SO4 to give 90% I (RR1 = R2R3 = O, R4 = R6 = H, R5 = Me). This was treated with LiAlH4 in Et2O-THF at room temp. to give 30% I (R = R3 = R4 = R6 = H, R1R2 = bond, R5 = Me) (II). II inhibited tetrabenazine-induced ptosis in mice with an ED50 of 0.3 mg/kg i.p.

IT 98159-29-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. and antidepressant activity of)

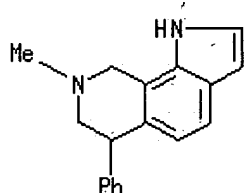
RN 98159-29-6 HCAPLUS

CN 1H-Pyrrolo[3,2-h]isoquinoline, 6,7,8,9-tetrahydro-8-methyl-6-phenyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

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CRN 98159-28-5

CMF C18 H18 N2

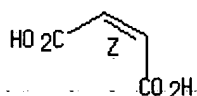


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



=> file reg

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

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TOTAL

SESSION

499.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.30	-5.21

FILE 'REGISTRY' ENTERED AT 06:58:15 ON 01 OCT 2003  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2  
DICTIONARY FILE UPDATES: 29 SEP 2003 HIGHEST RN 595542-94-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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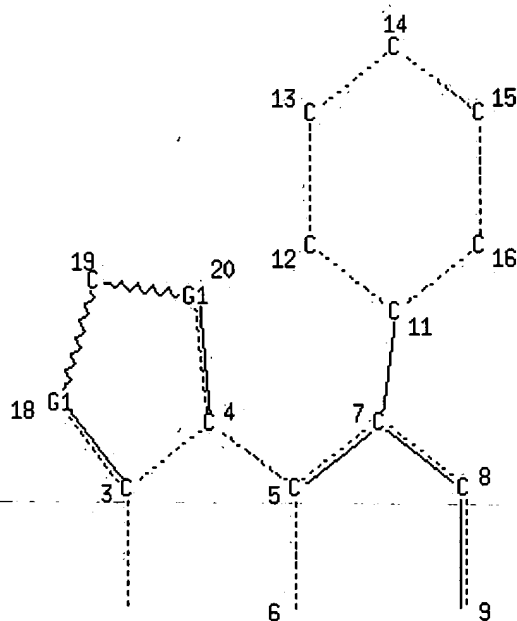
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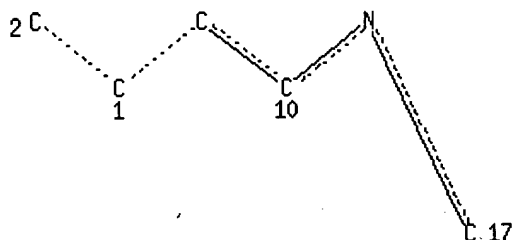
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Page 1-A



Page 1-B



Page 2-B

VAR G1=21/22/23/24

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DEFAULT MLEVEL IS ATOM  
MLEVEL IS CLASS AT 17  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 11

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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100.0% PROCESSED 330 ITERATIONS

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SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 5511 TO 7689

PROJECTED ANSWERS: 1 TO 80

L18 1 SEA SSS SAM L17

=> s 117 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

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 FULL SCREEN SEARCH COMPLETED - 6837 TO ITERATE

100.0% PROCESSED 6837 ITERATIONS  
 SEARCH TIME: 00.00.01

22 ANSWERS

L19 22 SEA SSS FUL L17

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

148.95

648.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-5.21

FILE 'HCAPLUS' ENTERED AT 07:00:08 ON 01 OCT 2003  
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FILE COVERS 1907 - 1 Oct 2003 VOL 139 ISS 14  
 FILE LAST UPDATED: 30 Sep 2003 (20030930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l19

L20 1 L19

=> d l20, ibib abs fhitr, 1

L20 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2002:51467 HCAPLUS

DOCUMENT NUMBER: 136:118393

TITLE: Preparation and use of furan-fused-4-phenyl substituted tetrahydroisoquinolines for treatment of attention deficit hyperactivity disorder (ADHD)

INVENTOR(S): Beck, James P.; Pechulis, Anthony D.; Harms, Arthur E.

PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

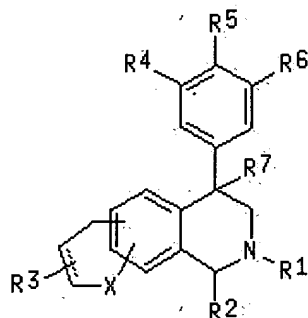
DOCUMENT TYPE: Patent

LANGUAGE: English

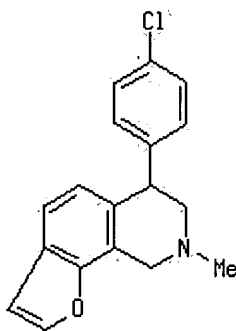
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2002004455</u>	A2	20020117	<u>WO 2001-US21818</u>	20010711
<u>WO 2002004455</u>	A3	20020620		
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<u>EP 1299393</u>	A2	20030409	<u>EP 2001-952616</u>	20010711
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
<u>BR 2001012350</u>	A	20030624	<u>BR 2001-12350</u>	20010711
<u>PRIORITY APPLN. INFO.:</u>			<u>US 2000-217412P</u>	P 20000711
			<u>WO 2001-US21818</u>	W 20010711
OTHER SOURCE(S):		MARPAT 136:118393		
GI				



I



II

AB Title compds. I [R1 = alk(en/yn)yl, cycloalkyl, 5-cycloalkylalkyl and benzyl, each of which is optionally substituted with 1 to 3 substituents; R2 = H, alk(en/yn)yl, cycloalkyl, cycloalkylalkyl and haloalkyl; R3 = H, halo, alkyl, haloalkyl and cycloalkyl, wherein alkyl, haloalkyl and cycloalkyl are optionally substituted with 1 to 3 substituents selected from alkoxy and amino; R4-6 = H, halo, alkoxy, NO<sub>2</sub>, amino, amido, ureido, S(O)<sub>n</sub>, CN, acyl, carboxy, carboxamide, alk(en/yn)yl, cycloalkyl and cycloalkylalkyl; alternatively R5-6 = O-alkyl-O; R7 = H, halo and alkoxy; X = O, NH (and substituted derivs.) and S; n = 0 - 2] with some provisos, were prepd. E.g., 7-formylbenzofuran was converted to the corresponding methylamino-Me deriv. (MeOH, MeNH<sub>2</sub>, NaBH<sub>4</sub>), alkylated with p-chlorophenacyl bromide (CH<sub>2</sub>Cl<sub>2</sub>, Et<sub>3</sub>N) and reduced to the amino alc. (CH<sub>2</sub>Cl<sub>2</sub>, NaBH<sub>4</sub>, 5 h, 0° → room temp.). This intermediate was treated dropwise with MsOH (CH<sub>2</sub>Cl<sub>2</sub>, 0°C → reflux, overnight) to give II as a yellow oil (18% overall yield). Over 150 synthetic examples were provided. Compds. I are selective neurotransmitter receptor binding ligands (no data). I are useful in the treatment of attention-deficit hyperactivity disorder.

IT 389845-09-4P

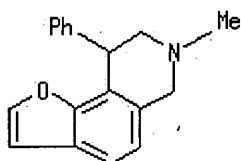


RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Préparation); USES (Uses)

(drug; prepn. and use of furan-fused-4-Ph substituted tetrahydroisoquinolines for treatment of attention deficit hyperactivity disorder (ADHD))

RN 389845-09-4 HCAPLUS

CN Furo[2,3-f]isoquinoline, 6,7,8,9-tetrahydro-7-methyl-9-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



# HCl

=> file caold

COST IN U.S. DOLLARS

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TOTAL

ENTRY

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FULL ESTIMATED COST

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655.67

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.65

-5.86

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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(FILE 'HOME' ENTERED AT 06:47:41 ON 01 OCT 2003)

FILE 'REGISTRY' ENTERED AT 06:47:47 ON 01 OCT 2003

L1 STRUCTURE UPLOADED

L2 42 S L1

L3 STRUCTURE UPLOADED

L4 0 S L3

L5 5 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 06:51:49 ON 01 OCT 2003

L6 5 S L5

L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 06:53:19 ON 01 OCT 2003

L8 STRUCTURE UPLOADED

L9 3 S L8

L10 31 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 06:53:43 ON 01 OCT 2003

L11 6 S L10

L12 1 S L11 NOT L6

FILE 'REGISTRY' ENTERED AT 06:54:59 ON 01 OCT 2003

L13 STRUCTURE UPLOADED

L14 8 S L13

L15 137 S L13 FULL

FILE 'HCAPLUS' ENTERED AT 06:56:51 ON 01 OCT 2003

L16 2 S L15

FILE 'REGISTRY' ENTERED AT 06:58:15 ON 01 OCT 2003

L17 STRUCTURE UPLOADED

L18 1 S L17

L19 22 S L17 FULL

FILE 'HCAPLUS' ENTERED AT 07:00:08 ON 01 OCT 2003

L20 1 S L19

FILE 'CAOLD' ENTERED AT 07:00:23 ON 01 OCT 2003

=> s 15

L21 0 L5

=> s 110

L22 0 L10

=> s 115

L23 0 L15

=> s 119

L24 0 L19

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.40

656.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

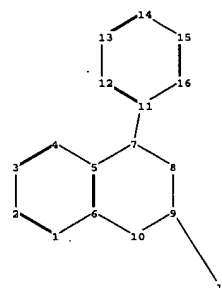
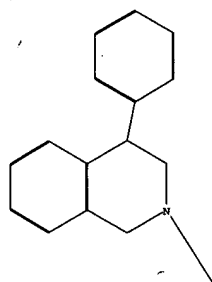
SESSION

CA SUBSCRIBER PRICE

0.00

-5.86

STN INTERNATIONAL LOGOFF AT 07:01:05 ON 01 OCT 2003



chain nodes :

17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

chain bonds :

7-11 9-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16

exact/norm bonds :

5-7 6-10 7-8 8-9 9-10 9-17

exact bonds :

7-11

normalized bonds :

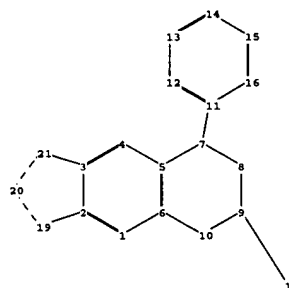
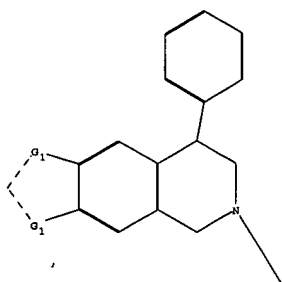
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

isolated ring systems :

containing 11 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS



chain nodes :

17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 19 20 21

chain bonds :

7-11 9-17

ring bonds :

1-2 1-6 2-3 2-19 3-4 3-21 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13  
13-14 14-15 15-16 19-20 20-21

exact/norm bonds :

2-19 3-21 5-7 6-10 7-8 8-9 9-10 9-17 19-20 20-21

exact bonds :

7-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

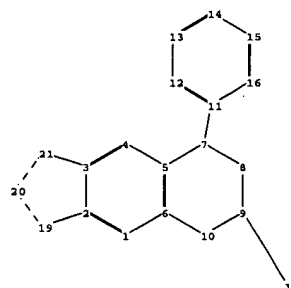
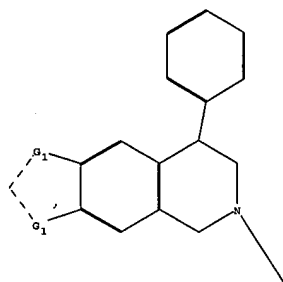
isolated ring systems :

containing 11 :

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom



chain nodes :

17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 19 20 21

chain bonds :

7-11 9-17

ring bonds :

1-2 1-6 2-3 2-19 3-4 3-21 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13  
13-14 14-15 15-16 19-20 20-21

exact/norm bonds :

2-19 3-21 5-7 6-10 7-8 8-9 9-10 9-17 19-20 20-21

exact bonds :

7-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

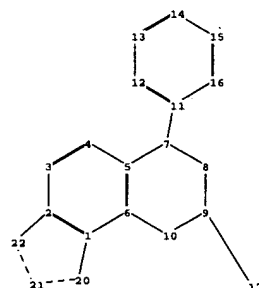
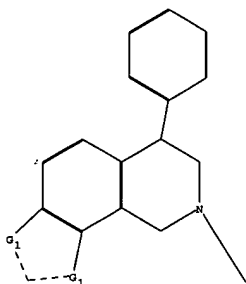
isolated ring systems :

containing 11 :

G1:O,S,N,C

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom



chain nodes :

17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 20 21 22

chain bonds :

7-11 9-17

ring bonds :

1-2 1-6 1-20 2-3 2-22 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13  
13-14 14-15 15-16 20-21 21-22

exact/norm bonds :

1-20 2-22 5-7 6-10 7-8 8-9 9-10 9-17 20-21 21-22

exact bonds :

7-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

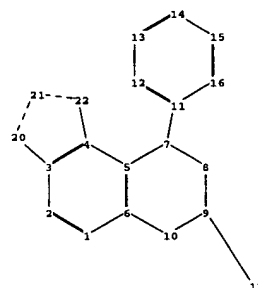
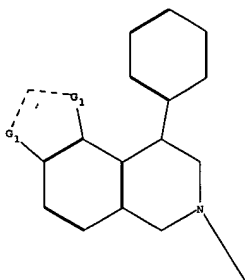
isolated ring systems :

containing 11 :

G1:O,S,N,C

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 20:CLASS 21:Atom 22:CLASS



chain nodes :

17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 20 21 22

chain bonds :

7-11 9-17

ring bonds :

1-2 1-6 2-3 3-4 3-20 4-5 4-22 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13  
13-14 14-15 15-16 20-21 21-22

exact/norm bonds :

3-20 4-22 5-7 6-10 7-8 8-9 9-10 9-17 20-21 21-22

exact bonds :

7-11

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

isolated ring systems :

containing 11 :

G1:O,S,N,C

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 20:Atom 21:Atom 22:Atom